

**Single-qubit operations in the double-donor structure
driven by strongly detuned optical pulses.**

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Abstract

We study theoretically the quantum dynamics of an electron in the singly-ionized double-donor structure in the semiconductor host under the influence of two strongly detuned laser pulses. This structure can be used as a charge qubit where the logical states are defined by the lowest two energy states of the remaining valence electron localized around one or another donor. The quantum operations are performed via Raman-like transitions between the localized (qubit) states and the manifold of states delocalized over the structure. The possibility of realization of arbitrary single-qubit rotations, including the phase gate, the NOT gate, and the Hadamard gate, is demonstrated. The advantages of the off-resonant driving scheme for charge qubit manipulations are discussed in comparison with the resonant scheme proposed earlier.

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I. INTRODUCTION

In view of recent progress in the development of the controlled-donor implantation techniques [1], Kane's paradigm of the solid-state quantum computations [2] has gained new insights. The alternative schemes using the orbital [3, 4] or spin [5, 6] degrees of freedom of the donor-bounded electrons to encode the quantum information instead of the nuclear donor spins, have been proposed. Besides, several refinements of the original proposal concerning the initialization [7] and read-out [8, 9, 10, 11] as well as the information transfer through the quantum networks [12, 13, 14] have been made.

In particular, the pair of donors sharing an electron has been considered as very promising candidate for the solid-state qubit embodiment [3]. The qubit is presented by the electron orbital states positioned at the different donors. There are two main driving mechanisms for the coherent electron evolution defining a quantum operation on such a qubit. First uses the electric fields through an application of the adiabatically switched voltages to the surface gates placed above the donor structure to modify the confinement potential, thus varying the electron tunnelling rates between neighboring donors [3, 15]. The desired state of the qubit is realized by an appropriate choice of the voltage parameters. The second scheme relies upon the optical dipole transitions between the size-quantized one-electron levels induced by the resonant pulses [16, 17]. As it was shown, an arbitrary single-qubit operation can be achieved with two simultaneously switched pulses connecting the qubit states

via the excitation of the state delocalized over the structure. The latter scheme is likely to be more preferable than the former due to its higher selectivity and lower field intensity. The successful implementation of the quantum operations, however, requires one to provide the high precision in the durations, the frequencies, the polarizations and the strengths of the pulses together with reliable control over the delay time and the phase difference between the pulses. Besides, the use of the intermediate state lying in the neighborhood of the continuum introduces the decoherence caused by the ionization and the spontaneous emission from this state.

Here we propose the way to overcome the difficulties inherent to the electron charge manipulations by optical means. We show that the off-resonant laser pulses can be used to generate an arbitrary rotation of the qubit-state vector as well as to drive an electron between the remote donors. It is essential that this method is based on the Raman-like transitions between the localized electron states of an effective molecular ion where the excited (delocalized over the double-donor system) states irrespective of their number are used as the transport channels. As we shall see, the coherent electron dynamics is described by the simple analytical model. The pulse and structure parameters needed for that type of quantum evolution may be evaluated from the results obtained in this study.

II. MODEL

We begin with the description of the one-electron double-donor (DD) structure (Fig. 1). Let the donors A and B be placed on the axis x from each other at

the distance R large enough to consider their ground orbital states, $|A0\rangle$ and $|B0\rangle$, to be isolated. Due to this fact those states may be used as the qubit states $|0\rangle$ and $|1\rangle$, respectively (if an electron is localized on the donor $A(B)$, the qubit is in the state $|0\rangle$ ($|1\rangle$)). The energy difference $\Delta = \varepsilon_{B0} - \varepsilon_{A0} \equiv \varepsilon_1 - \varepsilon_0$ may be introduced due to the structure asymmetry caused by the fabrication process and/or by the bias voltages V applied to the donors. The coupling between the excited states of the donors through the electron tunnelling gives rise to the forming of hybridized states delocalized over the DD structure. However, if $R \gg a_B$ (a_B is the effective Bohr radius of host material) the low-lying excited states are hybridized weakly and do not participate the two-donor dynamics. We will consider therefore only the excited states of individual donors whose orbitales considerably overlap, e.g., the $|nP_x\rangle$ states. The resulting effective single-electron spectrum of the DD structure is presented by the sequence of the states $\{|k\rangle\}_{exc}$ which for $\Delta = 0$ are the doublets composed of the symmetric and antisymmetric superpositions of isolated donor states. If $\Delta \neq 0$, the spectrum is expected to be much more complex. Taking into account the hydrogen-like spectrum of the isolated donors we expect the excited states close to the edge of the potential barrier separating the donors to have the quasi-continuous energy distribution. The energy gap $\omega_{exc} = \varepsilon_{exc}^{\min} - \varepsilon_1$ between the state $|1\rangle$ and the lowest state $|k\rangle_{exc}^{\min}$ from that manifold is assumed to be greater than all other energy scales relevant for consideration:

$$\omega_{exc} > \Delta, \quad \omega_{exc} > \max \Delta_{mn}, \quad \Delta_{mn} = |\varepsilon_m - \varepsilon_n|, \quad m, n \in \{k\}_{exc}. \quad (1)$$

In what follows we shall study the one-electron quantum dynamics involving the localized (qubit) states, $|0\rangle$ and $|1\rangle$, and the states $\{|k\rangle\}_{exc}$ delocalized over the structure. Our aim is to choose the field and structure parameters so that to drive an initial qubit state $|\Psi(t_0)\rangle = \alpha_0|0\rangle + \beta_0|1\rangle = (\alpha_0, \beta_0)^T$ into the final state $|\Psi(t)\rangle = \alpha|0\rangle + \beta|1\rangle = (\alpha, \beta)^T$ with the desired coefficients α and β .

In the absence of an external field the DD structure is characterized by the stationary Hamiltonian H_0 with the eigenstates $\{|k\rangle\}$ and the eigenenergies $\{\varepsilon_k\}$:

$$H_0 |k\rangle = \varepsilon_k |k\rangle. \quad (2)$$

The eigenstates $\{|k\rangle\}$ form the complete orthonormal set so that

$$\sum_k |k\rangle \langle k| = 1. \quad (3)$$

In the presence of the electromagnetic field the system Hamiltonian reads

$$H = H_0 - e\mathbf{E}(t) \mathbf{r}, \quad (4)$$

where e is the electron charge, $\mathbf{E}(t)$ is the field strength, \mathbf{r} is the radius-vector of an electron. With the help of Eqs. (2) and (3) we rewrite the Eq. (4) in terms of the projection operators:

$$H = \left(\sum_k |k\rangle \langle k| \right) H \left(\sum_m |m\rangle \langle m| \right) = \sum_k \varepsilon_k |k\rangle \langle k| + \mathbf{E}(t) \sum_{k,m} \mathbf{d}_{km} |k\rangle \langle m|, \quad (5)$$

where $\mathbf{d}_{km} = \langle k| - e\mathbf{r} |m\rangle$ is the matrix element of optical dipole transition between the states $|k\rangle$ and $|m\rangle$. The state vector of the system may be presented in the form

$$|\Psi(t)\rangle = \sum_n c_n(t) e^{-i\varepsilon_n t} |n\rangle \quad (6)$$

and is governed by the non-stationary Schrödinger equation

$$i\frac{\partial |\Psi(t)\rangle}{\partial t} = H |\Psi(t)\rangle, \quad (7)$$

with the initial condition $|\Psi(t_0)\rangle = \alpha_0 |0\rangle + \beta_0 |1\rangle$ (hereafter $\hbar \equiv 1$).

Inserting Eqs. (5) and (6) into Eq. (7) we arrive at the set of linear differential equations for the probability amplitudes $c_n(t)$. We shall only examine the transitions between the states $|0\rangle$ and $|1\rangle$ and the states $\{|k\rangle\}_{exc}$:

$$\begin{cases} i\dot{c}_0 = \mathbf{E}(t) \sum_k \mathbf{d}_{0k} c_k e^{-i\omega_{0k}t} \\ i\dot{c}_1 = \mathbf{E}(t) \sum_k \mathbf{d}_{1k} c_k e^{-i\omega_{1k}t} \\ i\dot{c}_k = \mathbf{E}(t) (\mathbf{d}_{0k}^* c_0 e^{i\omega_{0k}t} + \mathbf{d}_{1k}^* c_1 e^{i\omega_{1k}t}), \quad k \in \{k\}_{exc}, \end{cases} \quad (8)$$

where $\omega_{0(1)k} = \varepsilon_k - \varepsilon_{0(1)}$.

Let the electromagnetic field imposed on the structure to have (in the dipole approximation) the form of two phase-locked pulses

$$\mathbf{E}(t) = \mathbf{E}_0(t) \cos(\omega_0 t + \varphi_0) + \mathbf{E}_1(t) \cos(\omega_1 t + \varphi_1), \quad (9)$$

where the pulse envelopes $\mathbf{E}_0(t) = \mathbf{E}_0 f_0(t)$, $\mathbf{E}_1(t) = \mathbf{E}_1 f_1(t)$ are the slowly-varying (compared to optical frequencies) time-dependent functions, $\omega_{0,1}$ are the pulse frequencies, and $\varphi_{0,1}$ are the pulse phases. We require both pulses to be in the two-photon resonance with the DD structure, i.e. $\varepsilon_0 + \omega_0 = \varepsilon_1 + \omega_1$ or, alternatively,

$$\delta_{0k} = \delta_{1k} \equiv \delta_k, \quad (10)$$

where $\delta_{0(1)k} = \omega_{0(1)} - \omega_{0(1)k}$ is the detuning of the pulse frequency $\omega_{0(1)}$ from the resonant frequency $\omega_{0(1)k}$.

Making use of the rotating-wave approximation we obtain from Eqs. (8) the following set:

$$\begin{cases} i\dot{c}_0 = \sum_k [\lambda_{0k}(t) + \mu_{1k}(t) e^{i\Delta t}] c_k e^{i\delta_k t} \\ i\dot{c}_1 = \sum_k [\mu_{0k}(t) e^{-i\Delta t} + \lambda_{1k}(t)] c_k e^{i\delta_k t} \\ i\dot{c}_k = [\lambda_{0k}^*(t) + \mu_{1k}^*(t) e^{-i\Delta t}] c_0 e^{-i\delta_k t} + \\ \quad + [\mu_{0k}^*(t) e^{i\Delta t} + \lambda_{1k}^*(t)] c_1 e^{-i\delta_k t}, \quad k \in \{k\}_{exc}, \end{cases} \quad (11)$$

where $\lambda_{0(1)k}(t) = \lambda_{0(1)k} f_{0(1)}(t) e^{i\varphi_{0(1)}}$, $\mu_{0(1)k}(t) = \mu_{0(1)k} f_{0(1)}(t) e^{i\varphi_{0(1)}}$, $\lambda_{0(1)k} = \mathbf{d}_{0(1)k} \mathbf{E}_{0(1)} / 2$, $\mu_{0(1)k} = \mathbf{d}_{1(0)k} \mathbf{E}_{0(1)} / 2$ and the identities $\omega_{0(1)} - \omega_{1(0)k} = \delta_{1(0)k} \mp \Delta$ are used.

Eqs. (11) describe the dynamical process involving many three-level excitation schemes that act in parallel. Each of them is characterized by the set of parameters Δ , $\lambda_{0(1)k}$, $\mu_{0(1)k}$, and δ_k , where $k \in \{k\}_{exc}$. We shall suppose the values of $\lambda_{0(1)k}$ and $\mu_{0(1)k}$ to be of the same order. Depending on the ratios between these parameters k -th excitation scheme may be classified in the following way. First we consider the case of small detunings. If the coupling coefficients of the optical dipole transitions $\lambda_{0(1)k}$ and the detunings δ_k satisfy the inequality

$$|\delta_k|, \Delta \ll |\lambda_{0k}|, |\lambda_{1k}|, \quad (12)$$

the three-level scheme works in the *resonant symmetric* regime. Instead, the applicability of the *resonant asymmetric* scheme [16] is provided by the condition

$$|\delta_k| \ll |\lambda_{0k}|, |\lambda_{1k}| \ll \Delta. \quad (13)$$

We see that the asymmetry/symmetry of the structure isn't defined by the presence/absence of the energy difference Δ only but by the ratio between Δ and the

coupling coefficients $|\lambda_{0k}|, |\lambda_{1k}|$ as well. In other words, a driven DD structure can be treated (relative to the k -th transition scheme) as symmetric if the influence of the parameter Δ introducing a "static" asymmetry is compensated by an appropriate value of the field strength defined from (12). In this case only one external pulse is sufficient to excite both transitions [18].

Next we shall examine the opposite case where the states $|0\rangle, |1\rangle$ are connected through the off-resonant transitions involving the manifold of the excited states lying at the edge of the potential barrier. Two situations are possible again, i.e.

$$\Delta \ll |\lambda_{0k}|, |\lambda_{1k}| \ll |\delta_k| \quad (14)$$

and

$$|\lambda_{0k}|, |\lambda_{1k}| \ll |\delta_k|, \Delta. \quad (15)$$

The first of these inequalities corresponds to the *off-resonant symmetric* excitation scheme. This situation was studied in Refs. [19, 20] for the double-dot structures. As it was shown, the set of single-qubit operations produced by such one-electron dynamics is incomplete since in order to realize an arbitrary rotation of the qubit-state vector the structure symmetry must be broken. Here our attention will be focused on the *off-resonant asymmetric* case for which the conditions (15) are satisfied and each pulse drives the transitions between only one of localized state $|0\rangle$ ($|1\rangle$) and the transport states $\{|k\rangle\}_{exc}$. This implies also that the values of Δ and δ_k must be rather different from each other for all k to prevent the single-donor resonant dynamics. It may be attained, e.g., by setting $\omega_0 < \omega_{exc}$.

III. THE OFF-RESONANT DYNAMICS

Using the inequalities (15) let us average each of equations (11) over the time interval $T_\Delta = 2\pi/\Delta$ on which all of the time-dependent functions except $\exp(\pm i\Delta t)$ may be replaced by their mean values [21] so that after integration we arrive at the following set of equations:

$$\begin{cases} i\dot{c}_0 = \sum_k \lambda_{0k}(t) b_k \\ i\dot{c}_1 = \sum_k \lambda_{1k}(t) b_k \\ i\dot{b}_k = -\delta_k b_k + \lambda_{0k}^*(t) c_0 + \lambda_{1k}^*(t) c_1, \quad k \in \{k\}_{exc}, \end{cases} \quad (16)$$

where $b_k = c_k \exp(i\delta_k t)$, $k \in \{k\}_{exc}$. The applicability of Eqs. (16) requires the pulse switching times $\tau_{0(1)sw}$ to be rather long as compared with T_Δ . The inequalities (15) allow one to apply the adiabatic elimination procedure [22] to the intermediate levels $\{|k\rangle\}_{exc}$:

$$\dot{b}_k \approx 0, \quad b_k \approx [\lambda_{0k}^*(t) c_0 + \lambda_{1k}^*(t) c_1] / \delta_k, \quad k \in \{k\}_{exc} \quad (17)$$

and equations for two remaining probability amplitudes c_0, c_1 in the matrix form read

$$i \frac{\partial}{\partial t} \begin{pmatrix} c_0 \\ c_1 \end{pmatrix} = \begin{pmatrix} \Lambda_0(t) & \Lambda_2(t) \\ \Lambda_2^*(t) & \Lambda_1(t) \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \end{pmatrix}, \quad (18)$$

where $\Lambda_0(t) = \Lambda_0 f_0^2(t)$, $\Lambda_1(t) = \Lambda_1 f_1^2(t)$, $\Lambda_2(t) = \Lambda_2 f_0(t) f_1(t)$ and $\Lambda_0 = \sum_k |\lambda_{0k}|^2 / \delta_k$, $\Lambda_1 = \sum_k |\lambda_{1k}|^2 / \delta_k$, $\Lambda_2 = e^{i(\varphi_0 - \varphi_1)} \sum_k \lambda_{0k} \lambda_{1k}^* / \delta_k$.

The eigenstates and the eigenenergies of the matrix in right-hand side of Eq. (18) may be written as

$$\begin{cases} |+\rangle = e^{i \arg[\Lambda_2(t)]} \cos[\Theta(t)/2] |0\rangle + \sin[\Theta(t)/2] |1\rangle \\ |-\rangle = e^{i \arg[\Lambda_2(t)]} \sin[\Theta(t)/2] |0\rangle - \cos[\Theta(t)/2] |1\rangle \end{cases} \quad (19)$$

and

$$E_{\pm}(t) = [\Lambda_0(t) + \Lambda_1(t)]/2 \pm \Omega(t), \quad (20)$$

respectively, where

$$\cos[\Theta(t)] = [\Lambda_0(t) - \Lambda_1(t)]/2\Omega(t), \quad \sin[\Theta(t)] = |\Lambda_2(t)|/\Omega(t), \quad (21)$$

and

$$\Omega(t) = \sqrt{[\Lambda_0(t) - \Lambda_1(t)]^2/4 + |\Lambda_2(t)|^2} \quad (22)$$

is the instantaneous Rabi frequency. Using the unitary transformation

$$D(t) = \begin{pmatrix} e^{i \arg[\Lambda_2(t)]} \cos[\Theta(t)/2] & e^{i \arg[\Lambda_2(t)]} \sin[\Theta(t)/2] \\ \sin[\Theta(t)/2] & -\cos[\Theta(t)/2] \end{pmatrix} \quad (23)$$

we represent the state vector in the instantaneous basis $\{|+\rangle, |-\rangle\}$ as

$$|\Phi(t)\rangle = a_+(t)|+\rangle + a_-(t)|-\rangle, \quad |\Psi(t)\rangle = D(t)|\Phi(t)\rangle \quad (24)$$

and rewrite Eq. (18) in the new basis as

$$i \frac{\partial}{\partial t} \begin{pmatrix} a_+ \\ a_- \end{pmatrix} = \begin{pmatrix} E_+ & \dot{\Theta}/2 \\ -\dot{\Theta}/2 & E_- \end{pmatrix} \begin{pmatrix} a_+ \\ a_- \end{pmatrix}, \quad (25)$$

where

$$\dot{\Theta}(t) = \frac{|\dot{\Lambda}_0(t) - \dot{\Lambda}_1(t)| |\Lambda_2(t)| - |\dot{\Lambda}_2(t)| |\Lambda_0(t) - \Lambda_1(t)|}{[\Lambda_0(t) - \Lambda_1(t)]^2/4 + |\Lambda_2(t)|^2}. \quad (26)$$

Here we restrict our interest by the diagonal evolution followed from the choice of the system parameters for which $\dot{\Theta}(t) \ll E_{\pm}(t)$. In this case the solution of Eq.

(25) is straightforward:

$$\begin{aligned} a_+(t) &= a_+(t_0) \exp \left[-i \int_{t_0}^t E_+(t') dt' \right], \\ a_-(t) &= a_-(t_0) \exp \left[-i \int_{t_0}^t E_-(t') dt' \right]. \end{aligned} \quad (27)$$

With the help of equations (23), (24), and (27) we may write down the expression for the evolution matrix of the qubit-state vector $|\Psi(t)\rangle$ in the laboratory frame:

$$\begin{aligned}
|\Psi(t)\rangle &= U |\Psi(t_0)\rangle, \\
U &= \begin{pmatrix} e^{-i\varepsilon_0 t} & 0 \\ 0 & e^{-i\varepsilon_1 t} \end{pmatrix} D(t) \begin{pmatrix} e^{-i \int_{t_0}^t E_+(t') dt'} & 0 \\ 0 & e^{-i \int_{t_0}^t E_-(t') dt'} \end{pmatrix} D^\dagger(t_0) = \\
&= e^{-i[\varepsilon_0 t + \varphi_\Lambda(t)]} \begin{pmatrix} u_{00} & u_{01} \\ u_{10} e^{-i\Delta t} & u_{11} e^{-i\Delta t} \end{pmatrix},
\end{aligned} \tag{28}$$

where

$$\begin{aligned}
u_{00} &= u_{11}^* = e^{-i\tilde{\Omega}(t)} \cos[\Theta(t)/2] \cos[\Theta(t_0)/2] + e^{i\tilde{\Omega}(t)} \sin[\Theta(t)/2] \sin[\Theta(t_0)/2], \\
u_{01} &= -u_{10}^* = \\
&= e^{i \arg[\Lambda_2(t)]} \left\{ e^{-i\tilde{\Omega}(t)} \cos[\Theta(t)/2] \sin[\Theta(t_0)/2] - e^{i\tilde{\Omega}(t)} \sin[\Theta(t)/2] \cos[\Theta(t_0)/2] \right\},
\end{aligned} \tag{29}$$

and

$$\tilde{\Omega}(t) = \int_{t_0}^t \Omega(t') dt', \quad \varphi_\Lambda(t) = \int_{t_0}^t [\Lambda_0(t') + \Lambda_1(t')]/2 dt'. \tag{30}$$

The expressions (28) - (30) describe the effective two-level dynamics that corresponds to the continuous evolution of the qubit state vector on the Bloch sphere. In the next section we show how to choose the pulse and structure parameters in order to realize the most important single-qubit gates.

IV. SINGLE-QUBIT OPERATIONS

We illustrate the qubit state engineering by considering a particular case of the driving pulses sharing the same time dependence, - i.e. $f_0(t) = f_1(t) \equiv f(t)$. The condition $\dot{\Theta} = 0$ is then satisfied and the components of the evolution matrix (28)

take the form

$$\begin{aligned} u_{00} &= u_{11}^* = \cos [\tilde{\Omega}(t)] - i \cos(\Theta_0) \sin [\tilde{\Omega}(t)], \\ u_{01} &= -u_{10}^* = -ie^{i \arg(\Lambda_2)} \sin(\Theta_0) \sin [\tilde{\Omega}(t)], \end{aligned} \quad (31)$$

where $\Theta_0 = \arcsin \left[|\Lambda_2| / \sqrt{(\Lambda_0 - \Lambda_1)^2 / 4 + |\Lambda_2|^2} \right]$. The dynamics described by the equations (31) is sufficient to generate an arbitrary single-qubit rotation on the Bloch sphere. For example, the quantum operations such as NOT (σ_x): $(\alpha_0, \beta_0)^T \rightarrow (\beta_0, \alpha_0)^T$; PHASE (σ_z): $(\alpha_0, \beta_0)^T \rightarrow (\alpha_0, -\beta_0)^T$; and Hadamard (H): $(\alpha_0, \beta_0)^T \rightarrow [(\alpha_0 + \beta_0)/\sqrt{2}, (\alpha_0 - \beta_0)/\sqrt{2}]^T$ can be realized (up to the common phase) given the following choices of the pulse - structure parameters:

$$\tilde{\Omega}(T) = \pi/2 + \pi k, \quad T\Delta = 2\pi l, \quad \arg(\Lambda_2) = 2\pi m \quad (32)$$

and

$$\Theta_0(\sigma_x) = \pi/2 + \pi n, \quad \Theta_0(\sigma_z) = \pi n, \quad \Theta_0(H) = \pi/4 + \pi n, \quad (33)$$

respectively. Here k, l, m , and n are the integers and T is the pulse duration. Of course, this is not a unique parameter choice to attain the above quantum operations. Let us evaluate the time T_{NOT} needed to implement NOT operation. For the pulse strengths $E_0 \sim E_1 \sim 10$ V/cm and $a_B \sim 3$ nm one has $|\lambda_{0k}| \sim |\lambda_{1k}| \sim ea_B E_0 \sim 10^{-5}$ eV. By setting $\delta_k \sim -10^{-4}$ eV, $k = k_{exc}^{min}$ that ensures the validity of Eqs. (14) and (15) for all k , we obtain $|\Lambda_0| \geq |\lambda_{0k}|^2 / |\delta_k| \sim 10^9$ s⁻¹. Hence, $T_{NOT} \sim \Lambda_0^{-1}$ is of order of nanoseconds. More careful estimation requires the detailed knowledge of the energy spectrum of DD structure and the values of $\lambda_{0(1)k}$.

Note that the complete population transfer between the qubit states, or NOT operation, requires that $\Lambda_0 = \Lambda_1$. This is naturally met for nearly symmetric DD structures where $\Delta \approx 0$ and $|\mathbf{d}_{0k}| \approx |\mathbf{d}_{1k}|$. In general, however, one should keep in mind that $|\mathbf{d}_{0k}| \neq |\mathbf{d}_{1k}|$ that makes the performing of the condition $\Lambda_0 = \Lambda_1$ very problematic. It seems then reasonable to point the other way for the population transfer based upon the pulse-shaped techniques. Such methods, e.g., the stimulated Raman adiabatic passage (STIRAP) [23], are very robust against the pulse/structure imperfections and would allow one to handle the quantum information carefully. The theory of the adiabatic population transfer via multiple intermediate states, including the off-resonant case, was presented in Ref. [24]. Note that for the pulses strongly detuned from the resonance, the time ordering is no more important since successful population transfer may be attained for both intuitive and counterintuitive pulse sequences. If initially $c_0(t_0) = 1$, $c_1(t_0) = 0$, the intuitive (counterintuitive) pulse ordering means that $\lim_{t \rightarrow t_0} [f_0(t)/f_1(t)] = \infty(0)$ and $\lim_{t \rightarrow T} [f_0(t)/f_1(t)] = 0(\infty)$ and, as it follows from Eq. (21), $\Theta(t_0) = 0(\pi)$, $\Theta(T) = \pi(0)$. The population transfer may be understood as the adiabatic temporal development of the eigenstate $|+\rangle$ ($|-\rangle$) for the intuitive (counterintuitive) pulse ordering. As it is seen from Eq. (29), the qubit state inversion is realized in the asymmetric DD structures if the conditions $\arg[\Lambda_2(T)] \pm \tilde{\Omega}(T) = \pi n$ and $T\Delta = \pi(2m+1)$ are fulfilled. The detailed analysis concerning the arrangement of the pulse shapes in STIRAP can be found elsewhere [23].

V. DISCUSSION

To provide more clarity in the understanding of the advantages of the charge qubit-state engineering presented above, let us compare the resonant and off-resonant excitation schemes. The resonant optical driving of the DD structure modelled by single three-level scheme has been studied in Refs. [16, 17]. In the case considered here a more complex dynamics can take place involving more than one three-level scheme. For example, if we tune the lasers on resonance with the transition between the logical subspace $\{|0\rangle, |1\rangle\}$ and a state $|r\rangle$, $r \in \{k\}_{exc}$ located near the top of the barrier, a number of states with the energies close to ε_r will be excited as well. This picture is quite expected in the hydrogen-like molecular ions for the high-lying states which energies are within the interval $\Delta\varepsilon_r \leq |\lambda_{0(1)r}|$. However, for the symmetric structure it means that there will be no transitions between the qubit states. It is because the excited states belonging to the same doublet are presented by the symmetric and antisymmetric superpositions of the excited states of isolated donors which, being excited simultaneously, interfere constructively on one donor and destructively on another one. As a consequence, the donors are excited independently. This effect becomes more significant as the interdonor distance R increases and the tunnel coupling between the donors decreases. When the energy splitting of the maximally-resolved doublet becomes comparable with the coupling coefficients of the optical dipole transitions, the process of the electron transfer between the donors is terminated. Note that the optically driven DD structure

will demonstrate the similar behavior if one of the pulses is short enough so that its duration is $T \leq 1/\Delta\varepsilon_r$ and thus it contains harmonics in the frequency range $\delta\omega \sim 1/T \geq \Delta\varepsilon_r$. Again, the states with the energies belonging to the interval $\Delta\varepsilon_r$ will be excited simultaneously giving rise to the electron transfer blockage just outlined.

The reliable resonant scheme thus deals with single transport state and is very sensitive to the pulse detuning from the resonance with that state. For example, the non-zero detuning always produces an amplitude error in NOT gate because of incomplete depopulation of the initial state when the pulse is off [18]. On the contrary, the use of the off-resonant pulses enables one to exploit the whole number of excited states. Moreover, we don't need to control the pulse frequencies with high accuracy since a small variation in the pulse detunings brings about an insignificant change in the Rabi frequency (30). The computational errors originated from the frequency renormalization can be corrected by the corresponding change in the pulse duration due to the smooth time dependencies of the probability amplitudes. The only requirement that must be followed closely for successful electron state manipulations is the Raman two-photon resonant condition (10).

The selectivity of the electron resonant transfer requires also a strict control over the pulse polarizations. The transport states in the molecular ion are formed through the hybridization of those individual donor states whose orbitales are extended along the axis x that coincides with the interdonor direction. Other states are hybridized

weakly and cannot assist efficiently in the electron dynamics. Their excitations are due to the pulse components polarized along the axes y and z . It amounts to the population leakage into the non-hybridized single-donor states with the energies lying in the close proximity to the energy of the transport state. Let us define the small angles γ_{ny} and γ_{nz} that characterize the deviations of the n -th pulse polarization from the axis x :

$$\mathbf{E}_n = \mathbf{E}_{nx} + \mathbf{E}_{ny} \cos(\pi/2 + \gamma_{ny}) + \mathbf{E}_{nz} \cos(\pi/2 + \gamma_{nz}), \quad (34)$$

$$|\gamma_{ny}|, |\gamma_{nz}| \ll 1, \quad n = 0, 1,$$

then the probability of successful implementation of the quantum operations is reduced by a factor of $w \sim 1 - \max(\gamma_{ny}^2, \gamma_{nz}^2)$. In the off-resonant case, the populations of those states remain negligibly small ($\sim |\lambda_{nk}|^2 / \delta_k^2$) and the corresponding channel of population leakage is blocked.

The important difference between the resonant and off-resonant schemes lies in the treatment of the decoherence problem. We know the relaxation rates from the transport state caused by the spontaneous photon/phonon emission during the resonant excitation [17] may be high enough to corrupt the qubit state. In the off-resonant scheme the population of the intermediate state(s) is negligible and the probability of relaxation is drastically reduced. The influence of the residual population of the intermediate state on the adiabatic electron transfer in the three-level scheme was examined in Ref. [25] for the gaussian pulses. It was shown that the error introduced by the spontaneous emission together with the error due to the non-adiabaticity are inversely proportional to the pulse detuning and can be made

small enough to allow the fault tolerant quantum computation.

In our model of the single-electron off-resonant transitions we don't consider in detail the spectrum of the DD structure. The classification of excited states used as the transport states as well as their wave functions are still to be determined. Besides, the participation of the continuum states in the electron dynamics has been completely ignored. These states, in principle, can also be used as transport channels and, at the same time, can bring about additional decoherence (see, e.g., [26]). Both of these issues will be the topics of further development of the model.

VI. CONCLUSIONS

In this paper we have considered the one-electron double-donor structure subjected to the action of two off-resonant electromagnetic pulses. Unlike the other systems proposed to serve as the potential candidates for the solid state optically-controlled qubits (double quantum dots, rf-SQUIDs), the double-donor structure is characterized by sufficiently high density of the bound states at the edge of the barrier that separates the donors. It means that the three-level resonant scheme proposed earlier to implement the desired qubit-state evolution may be unsuitable to maintain the appropriate selectivity of the optical excitations. On the other hand, the off-resonant scheme seems to be more efficient for the qubit manipulations and robust in comparison with the resonant scheme. Though the Raman evolution of the qubit is slower than that in the case of the resonant driving, it seems to be more reliable for the realization of quantum operations. We have shown that the basic

single-qubit operations may be performed on the DD structure for several pulse and structure parameter choices. The use of the adiabatic schemes is of the particular interest.

It is also very important that we can operate on the qubit without the detailed knowledge of the spectral properties of the DD structure. Keeping the frequencies of the detuned pulses smaller than the difference between the energy of the lowest state of the excited manifold and the energy of the qubit state $|1\rangle$, we automatically use all states from that manifold as the transport states. The information about the structure and pulse parameters is contained in the Rabi frequency of the two-level oscillations. This frequency can be defined experimentally for each set of the detunings, the strengths, and the durations of the pulses. The results of those measurements could be used to reconstruct the features of the spectrum of the DD structure.

Note that the method of the electron-state manipulations by optical means can be applied also to the spin-based encoding schemes like that of Ref. [2]. The implementation of optically controlled effective electron spin exchange described in Ref. [27] for the two-electron double-dot structure, can be generalized on the two-electron DD structure.

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Fig. 1. Schematics of the quantum state manipulation in the one-electron double-donor structure. The qubit states $|0\rangle$ and $|1\rangle$ are defined by the localized orbital states of the donors A and B with the energies ε_0 and ε_1 , respectively. They are coupled by two optical pulses with the frequencies ω_0 and ω_1 being in the two-photon resonance ($\varepsilon_0 + \omega_0 = \varepsilon_1 + \omega_1$). The pulses are detuned from the excited (delocalized over the structure) state $|k\rangle$ by the detuning δ_k . The energy difference $\Delta = \varepsilon_1 - \varepsilon_0$ is introduced by the voltage $V > 0$ applied to the gate on the left of the structure.

